Quantum Control Theory for State Transformations:
Dark States and their Enlightenment

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For many quantum information protocols such as state transfer, entanglement transfer and entanglement generation, standard notions of controllability for quantum systems are too strong. We introduce the weaker notion of accessible pairs, and prove an upper bound on the achievable fidelity of a transformation between a pair of states based on the symmetries of the system. A large class of spin networks is presented for which this bound can be saturated. In this context, we show how the inaccessible dark states for a given excitation-preserving evolution can be calculated, and illustrate how some of these can be accessed using extra catalytic excitations. This emphasizes that it is not sufficient for analyses of state transfer in spin networks to restrict to the single excitation subspace. One class of symmetries in these spin networks is exactly characterized in terms of the underlying graph properties.

I. INTRODUCTION

The holy grail of quantum information is the realization of a universal quantum computer, capable of solving a variety of tasks, including some that cannot be solved efficiently by classical computers. Although progress has been made towards this goal, it remains a daunting task. A more practical alternative is to develop utility modules capable of specific tasks such as quantum wires for state transfer [1, 2] or entanglement generation [2–4], which are easier to design and manufacture. These tasks can be achieved with minimal or no control. Perfect state transfer, for example, can be achieved by propagation along a spin chain with a suitably engineered Hamiltonian [1, 2]. However, these schemes have obvious drawbacks such as the requirement for precise Hamiltonian engineering, and the fact that they are limited to performing a single fixed task. We would like to relax the constraints slightly and see how much is gained by adding a small amount of control. Do we enlarge the range of tasks that can be achieved and the systems that can be used?

Recent work suggests that it is indeed possible to vastly increase the potential of many systems with very limited control. Control of a single coupling and some local control of the end spins, for example, can be sufficient to efficiently realize a universal quantum computer [5, 6]. The problem of realizing quantum information primitives such as state transfer and entanglement generation using a minimal degree of control, and the related task of identifying the key properties of a system such that those control techniques can then be applied, have also been studied, in particular for spin systems. Most studies have focused on special geometries, particularly chains and quasi-one-dimensional systems [1–5, 7–9], dual-chains [10] and rings [11], but there have been some studies more general networks [12, 13]. Each of these investigations has proved a certain information processing property, but a general framework for determining the capability of an arbitrary network is still lacking.

In this paper, we propose a unifying framework for describing certain state transformation tasks that involve simultaneously transforming a fixed set of initial states into a fixed set of output states. This allows us to simultaneously discuss processing tasks such as perfect state transfer and entanglement generation, rather than tackle each case separately. These tasks require far less than full control of the system, but the ability to perform them is restricted by symmetries of the system. In Sec. II we discuss the notions of full controllability, and introduce the much weaker notion of sets of accessible pairs, and describe the role of Lie algebra symmetries, deriving bounds on the fidelity with which a given state transformation task can be realized based on symmetry properties of the system and control Hamiltonians. In Sec. III we demonstrate how the upper bounds on a state transformation task can be achieved within a large class of spin networks by controlling a single coupling between two spins. This includes an exact description of one class of symmetries for these systems, a necessary and sufficient condition for their presence being that the underlying network topology should correspond to a bipartite (two-colorable) graph. In Sec. IV it is shown how symmetry restrictions can be overcome by catalytic excitations, which emphasizes a marked difference in state transformation capabilities in comparison to the standard assumptions made in the analysis of state transfer in networks [31]. Finally, in Sec. V, we discuss how many of the important parameters for the transfer can be estimated from experimental data if they are not previously known.

II. SYMMETRIES & ACCESSIBLE STATES

A. Controllability

Among the most elementary concepts in control theory are reachability and controllability. Given a controlled dynamical system, a state $\mathbf{x}_1$ is *reachable* from an initial state $\mathbf{x}_0$ if there exists a control sequence and some time T such that the corresponding trajectory of the system

satisfies $\mathbf{x}(0) = \mathbf{x}_0$ and $\mathbf{x}(T) = \mathbf{x}_1$, and the system is *controllable* if any state in the state space is reachable from any other state [32]. Applied to bilinear control systems evolving on a Lie group, one can derive explicit criteria for controllability in terms of the Lie algebra formed by the dynamical generators. In particular, this is the case for decoherence-free quantum systems governed by the Schrödinger equation $\dot{U}(t) = -iH(t)U(t)$, where $U(t)$ is a unitary operator on the Hilbert space $\mathcal{H}$ of the system, and $H(t)$ is a Hamiltonian that depends linearly on a set of (real-valued) controls $f_m(t)$

$$H(t) = H_0 + \sum_m H_m f_m(t). \tag{1}$$

Here H_0 is the system Hamiltonian and the H_m are Hamiltonians governing the interaction with time-varying control fields $f_m(t)$. iH_0 and iH_m are the generators of the dynamics and they generate the *dynamical Lie algebra L*, which consists of all linear combinations and iterated commutators of these generators. For a system with Hilbert space dimension n the generators iH_m, $m = 0, 1, \ldots$, are anti-Hermitian matrices and thus can, at most, generate a subalgebra of the Lie algebra $\mathfrak{u}(n)$ of anti-Hermitian $n \times n$ matrices. A necessary and sufficient condition for the system (1) to be fully controllable then is the Lie algebra rank condition [14], $L \simeq \mathfrak{u}(n)$. If it is satisfied, then it can be shown that for any sufficiently large T, there exists a set of controls $f_m(t)$ such that any desired unitary gate $U_{\text{targ}} \in \mathfrak{U}(n)$ can be realized, i.e., given any $U_{\text{targ}} \in \mathfrak{U}(N)$, we have [15]

$$U_{\text{targ}} = U(T) = \exp_+ \left\{ -i \int_{t=0}^{T} H_0 + \sum_m f_m(t) H_m \, dt \right\}, \tag{2}$$

where $\exp_+$ denotes a positive time-ordered exponential. The reachable set $K = \exp(L)$, known as the *dynamical Lie group* is, in this case, the entire unitary group $\mathfrak{U}(n)$. Applied to an N-qubit system with a control-linear Hamiltonian (1), this implies that the system is fully controllable if and only if $L = \mathfrak{u}(2^N)$, and the corresponding dynamical Lie group $K = \mathfrak{U}(2^N)$. In practice, this condition can be slightly relaxed as we can usually neglect the global phase of the system, in which case $L = \mathfrak{su}(n)$ suffices, where $\mathfrak{su}(n)$ is the Lie algebra of trace-zero anti-Hermitian $n \times n$ matrices. In this paper we consider systems which are not fully controllable, for which L need not be $\mathfrak{u}(n)$ or $\mathfrak{su}(n)$.

B. Sets of Accessible Pairs

The main task in which we are interested throughout this paper is whether a system described by Eqn. (1) can be caused to transform its initial state $|\psi_{\text{in}}\rangle$ into a given target state $|\psi_{\text{targ}}\rangle$ through suitable manipulations of the control fields $f_m(t)$. If this is the case, we say $(|\psi_{\text{in}}\rangle, |\psi_{\text{targ}}\rangle)$ is an *accessible pair* of the system. If a given pair is not accessible then we quantify how well the system can achieve the desired transformation by calculating the fidelity of the optimal output state $|\psi_{\text{out}}\rangle$,

$$F := |\langle \psi_{\text{out}} | \psi_{\text{targ}} \rangle|^2.$$

Accessible pairs have $F = 1$, whereas a state is dark with respect to a given input if $F = 0$. One can extend this concept to sets of accessible pairs. We say a system has a set of (simultaneously) accessible pairs $\left\{ (|\psi_{\text{in}}^1\rangle, |\psi_{\text{targ}}^1\rangle), (|\psi_{\text{in}}^2\rangle, |\psi_{\text{targ}}^2\rangle) \right\}$ if the state $|\psi_{\text{in}}^1\rangle$ can be transformed into $|\psi_{\text{targ}}^1\rangle$ by some set of manipulations, and the same set of manipulations, in the same time, also transforms $|\psi_{\text{in}}^2\rangle$ into $|\psi_{\text{targ}}^2\rangle$.

This formalism provides a simple way for describing state transfer. Consider two nodes of a network A and B. State transfer from A to B can be achieved if

$$\{ (|0\rangle_A |\phi\rangle, |\psi\rangle |0\rangle_B), (|1\rangle_A |\phi\rangle, |\psi\rangle |1\rangle_B) \}$$

are accessible pairs for any arbitrary states $|\phi\rangle$ and $|\psi\rangle$ as it implies

$$(\alpha |0\rangle_A + \beta |1\rangle_A) |\phi\rangle \mapsto |\psi\rangle (\alpha |0\rangle_B + \beta |1\rangle_B)$$

for any superposition $\alpha |0\rangle + \beta |1\rangle$ (In this paper, we will only consider the decoherence-free case, which permits us to use linearity of the transformation task). Previous studies have focused almost exclusively on systems with excitation-preserving Hamiltonians because this vastly simplifies the task. As $|0\rangle^{\otimes N}$ is an eigenstate of such a system, setting $|\phi\rangle = |\psi\rangle = |0\rangle^{\otimes N-1}$ shows that we simply require that the system has an accessible pair $(|1\rangle_A |0\rangle^{\otimes N-1}, |0\rangle^{\otimes N-1} |1\rangle_B)$. We also mention that if we have an initial state $\frac{1}{\sqrt{2}} (|00\rangle + |11\rangle)_{A,A'} |\phi\rangle$, where A' is an ancilla qubit not part of the system, then the same accessible set as for state transfer allows the entanglement to be distributed between A' and B, $\frac{1}{\sqrt{2}} (|00\rangle + |11\rangle)_{B,A'} |\psi\rangle$.

The concept of accessible pairs is a very weak property compared to full controllability. It requires only that we can implement *one* unitary operator that simultaneously maps the input states $|\psi_{\text{in}}^k\rangle$ to the target states $|\psi_{\text{targ}}^k\rangle$, as opposed to an *arbitrary* unitary operator. In the example above, this means we only need to generate one unitary operator U that maps $|10\cdots0\rangle$ to $|00\cdots01\rangle$ to swap the quantum states of the first and last qubit. A one-dimensional Lie algebra may suffice for these purposes [1].

C. Reducibility and commuting symmetries

The most important reason for lack of full controllability of a control system on a Lie group are symmetries restricting the dynamical Lie algebra and dynamical Lie group. The relation between symmetries in the Hamiltonian of the system, irreducibility and loss of full control has been studied in recent papers by Polack *et al.* [16] and Sander *et al.* [17]. Lie algebra symmetries can be

classified in various ways. We shall distinguish between symmetries that imply reducibility of the dynamical Lie algebra and other symmetries.

A dynamic Lie algebra L is said to be *reducible* if it can be written as the direct sum of simple Lie algebras, e.g., $L \simeq \oplus_i L_i$. A necessary and sufficient condition for reducibility of L is the existence of a non-trivial Hermitian symmetry operator J that commutes with every element of L,

$$[H_m, J] = 0, \quad \forall\, m = 0, 1, 2, \ldots .$$

We shall refer to such J as *commuting symmetry operators* (CSOs). The commutation relations imply that the Hamiltonians leave non-trivial subspaces of the Hilbert space $\mathcal{H}$ invariant, and thus there exists a basis with respect to which J and all H_m have the same non-trivial block-diagonal structure, and we can write the Hilbert space $\mathcal{H}$ as a direct sum of mutually invariant subspaces $\mathcal{H} = \oplus_{d=1}^{D} \mathcal{H}_d$, where K is the number of independent blocks. Every H_m has an eigenvector decomposition such that every eigenvector can be written as a linear superposition of the eigenvectors of J drawn from a given degenerate eigenspace. The evolution on each subspace is described by its own Hamiltonian and thus the projection of a state onto each subspace, $\|\Pi_d \psi(t)\|$, is a constant of motion. Therefore, a necessary condition for a system to have an accessible pair $(|\psi_{\text{in}}\rangle, |\psi_{\text{targ}}\rangle)$ is that the initial state $|\psi_{\text{in}}\rangle$ and target state $|\psi_{\text{targ}}\rangle$ have the same projections onto each invariant subspace.

An important subclass of CSOs are the *permutation symmetries*, corresponding to the interchange of indistinguishable physical qubits of the N-qubit system. This particular subclass was referred to as an outer symmetry in [17]. A general procedure to find CSO is described in Appendix A.

D. Irreducibility and other symmetries

Irreducibility of the Lie algebra on an n-dimensional subspace $\mathcal{H}_k$ alone, however, is insufficient to ensure full controllability on this subspace. Assuming the Hamiltonians H_m are traceless, which can be achieved by subtracting a multiple of the identity if necessary, all irreducible components of the Lie algebra must be simple subalgebras of $\mathfrak{su}(n)$, which restricts to candidates of the form $\mathfrak{sp}(k)$, $\mathfrak{so}(k)$, $\mathfrak{su}(k)$ (for some $k < n$) or one of the exceptional Lie algebras. In this case, although we can always produce a unitary evolution that takes an initial state to a final state with a non-zero overlap with our target state, we may not be able to produce arbitrarily high overlap with the target [16]. For a subspace of dimension n this occurs precisely when the dynamical Lie algebra is neither $\mathfrak{su}(n)$ nor $\mathfrak{sp}(\frac{n}{2})$ [18].

Example 1: A simple example is a system with

$$H_0 = \frac{\omega}{2}\begin{pmatrix} -1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix}, \quad H_1 = \begin{pmatrix} 0 & d & 0 \\ d & 0 & d \\ 0 & d & 0 \end{pmatrix}.$$

The Lie algebra generated by $\{iH_0, iH_1\}$ is a unitary representation of $\mathfrak{so}(3)$ and indecomposable, but the system possesses an orthogonal symmetry; both matrices anticommute with

$$\begin{pmatrix} 0 & 0 & 1 \\ 0 & -1 & 0 \\ 1 & 0 & 1 \end{pmatrix}.$$

Let us define the basis to be $|\pm\lambda\rangle$ and $|1\rangle$, where $|\pm\lambda\rangle$ are the eigenvectors of H_0 with eigenvalues ± 1 respectively. H_1 couples the state $|1\rangle$ equally to the states $|\pm\lambda\rangle$, which are not directly coupled. Imagine we start from the state $|1\rangle$ and wish to produce a state $|\Psi\rangle$. The symmetry prevents us from perfectly producing $|\Psi\rangle$ unless

$$|\langle\lambda|\Psi\rangle| = |\langle -\lambda|\Psi\rangle|.$$

To see this, consider the unitary basis change

$$B = \frac{1}{2}\begin{pmatrix} 1 & \sqrt{2}i & 1 \\ \sqrt{2}i & 0 & -\sqrt{2}i \\ 1 & -\sqrt{2}i & 1 \end{pmatrix},$$

which maps the generators iH_0 and iH_1 onto real skew-symmetric matrices. Hence the evolution under any control sequence

$$B \exp_+ \left\{ -i \int_{t=0}^{T} H_0 + f(t)H_1 dt \right\} B^\dagger$$

must be described by a unitary matrix which is real. Since $B|1\rangle$ is a real vector (up to a global phase), the output $B|\Psi\rangle$ must be a real vector $(a, b, c)^T$. Hence, inverting B shows that we have $\langle \pm\lambda|\Psi\rangle = \frac{1}{2}(a + c \mp \sqrt{2}ib)$ which, because each of the coefficients is real, have equal magnitudes of amplitude.

Thus, given a maximal decomposition of the Hilbert space and Lie algebra into irreducible subalgebras, the next step is to identify symmetries such as orthogonal or symplectic symmetries, which are characterized by the existence of an orthogonal or symplectic symmetry operator J such that every element x in the irreducible Lie algebra L_i satisfies

$$x^T J + Jx = 0. \tag{3}$$

If all the dynamic generators of the system are of the form $x = iH_m$, where H_m are real-symmetric matrices, then $(iH_m)^T J + J(iH_m) = 0$ simplifies to the anticommutation relation

$$\{H_m, J\} = 0 \quad \forall m = 0, 1, 2, \ldots \tag{4}$$

and we shall therefore refer to such J as *anticommuting symmetry operators* (ASOs). Given the Hamiltonians H_m, such symmetries can easily be determined, as described in Appendix A.

1. Simultaneous Symmetries

A given system may have several CSOs that do not commute with each other, meaning that block-diagonal structures are not simultaneously realizable. We will always choose to analyze the symmetries that are most natural for the problem at hand, but one might worry that other non-commuting symmetries, be they CSOs or ASOs, could come into play. We will briefly justify that they do not, and therefore once we have picked a set of CSOs, we only have to find other CSOs or ASOs that act on the reduced space.

Imagine that we have found a CSO such that the system Hamiltonian and the control Hamiltonians all decompose into the same subspace structure,

$$\mathcal{H} = \mathcal{H}_1 \oplus \mathcal{H}_2$$

and that our initial state only has support on $\mathcal{H}_1$. Clearly, the evolution of that initial state is only determined by Hamiltonians restricted to $\mathcal{H}_1$; it does not matter what the Hamiltonians are on the complement to that space. So, let's say we have now found an M which could either be a CSO or ASO, but does not respect the subspace structure i.e. it couples between the two. The existence of this M must depend heavily on the structure of the Hamiltonians on the complement space – if they were different, M would not exist, and then it certainly couldn't restrict the dynamics within $\mathcal{H}_1$. Since we've argued, however, that our evolution of a state supported on $\mathcal{H}_1$ should not be affected by changing the Hamiltonians on the complement space, it must be that M does not affect the dynamics.

E. Maximum information transfer fidelity

Combining the knowledge of how the system Hamiltonian decomposes under basis change with the knowledge of the symmetries satisfied by each subsystem allows us to characterize what properties of the system's population are conserved under controlled evolution. This information can be used to calculate the maximum achievable overlap of an initial state with a target state as a measure of a network's suitability for certain information transmission and state preparation tasks.

First, let $\{|\phi_{\text{in}}\rangle\}$ be an orthonormal set of input states (we will typically take these to be determined by the subspace structure induced by the CSOs), which we can use to decompose the input state

$$|\psi_{\text{in}}\rangle = \sum_n \alpha_n |\phi_{\text{in}}^{(n)}\rangle.$$

Now suppose we can implement a particular unitary operator U that maps this set to a set of output states $U|\phi_{\text{in}}^{(n)}\rangle = |\phi_{\text{out}}^{(n)}\rangle$. Expressing the target state in this basis, we have

$$|\psi_{\text{targ}}\rangle = \sum_n \beta_n |\phi_{\text{out}}^{(n)}\rangle$$

whereas U can only transform $|\psi_{\text{in}}\rangle$ to

$$|\psi_{\text{out}}^U\rangle = \sum_n \alpha_n |\phi_{\text{out}}^{(n)}\rangle,$$

giving a maximum overlap with the target state of

$$F = |\langle \psi_{\text{out}}^U | \psi_{\text{targ}}\rangle|^2 = \left| \sum_{n,m} \alpha_m^* \beta_n \right|^2. \tag{5}$$

If $K = \exp(L)$ is the dynamical Lie group of the system, L being its dynamical Lie algebra, then the maximum transfer fidelity is

$$F = \max_{U \in K} |\langle \psi_{\text{out}}^U | \psi_{\text{targ}}\rangle|^2. \tag{6}$$

The latter expression is not easy to evaluate in general, but we can give upper bounds based on our knowledge of the symmetries of the system.

For example, suppose we know that the system decomposes due to the presence of CSOs, i.e., $\mathcal{H} = \bigoplus_d \mathcal{H}_d$ with $\dim \mathcal{H}_d = N_d$ and $\sum_d N_d = N$, and the dynamics on each subspace $\mathcal{H}_d$ are independent. We have

$$|\psi_{\text{in}}\rangle = \sum_d \Pi_d |\psi_{\text{in}}\rangle = \sum_d \alpha_d |\phi_{\text{in}}^{(d)}\rangle$$
$$|\psi_{\text{targ}}\rangle = \sum_d \Pi_d |\psi_{\text{targ}}\rangle = \sum_d \beta_d |\phi_{\text{out}}^{(d)}\rangle$$

where $\alpha_d = \|\Pi_d \psi_{\text{in}}\|$, $\beta_d = \|\Pi_d \psi_{\text{targ}}\|$ and $|\phi_{\text{in}}^{(d)}\rangle = \alpha_d^{-1} \Pi_d |\psi_{\text{in}}\rangle$, $|\phi_{\text{out}}^{(d)}\rangle = \beta_d^{-1} \Pi_d |\psi_{\text{targ}}\rangle$ are the respective (normalized) projections onto the subspaces. As any vector in the subspace $\mathcal{H}_d$ must remain in this subspace and the norm is preserved under unitary evolution, the best we can hope for is to simultaneously map the normalized states $|\phi_{\text{in}}^{(d)}\rangle$ onto $|\phi_{\text{out}}^{(d)}\rangle$ for all d, in which case we obtain

$$F = \left| \sum_d \alpha_d^* \beta_d \right|^2, \tag{7}$$

which is equivalent to (5). This bound is guaranteed to be attainable only if all the relative phases between subspaces can be controlled, i.e., if the dynamical Lie algebras on the subspaces are $\mathfrak{u}(N_d)$ or $\mathfrak{sp}(N_d/2) \oplus \mathfrak{u}(1)$. In practice, if the subspace Hamiltonians have zero trace then we do not have (subspace) phase controllability, and the most we can actually hope for is to map each $|\phi_{\text{in}}^{(d)}\rangle$ to a state $e^{i\phi_d}|\phi_{\text{out}}^{(d)}\rangle$, in which case we obtain the modified bound $F = \left| \sum_d \alpha_d^* \beta_d e^{i\phi_d} \right|^2$ and the original bound may be unattainable. Similarly, this may be the case if the subspace dynamics is constrained by further ASOs. Nonetheless the bound is often attainable for certain initial and target states even in spite of these symmetries and phase constraints.

III. APPLICATION TO SPIN NETWORKS

To demonstrate some of these concepts, we take the well-known class of examples as defined by the XX-coupled N-spin networks.

Define a graph $G_0 = (V_0, E_0)$ of the spin network, where V_0 is the vertex set (of N elements) of physical qubits and the edge set $E_0 = \{(i,j)|$qubit i interacts directly with qubit $j\}$. The system Hamiltonian for the spin network is thus

$$H_0 := \frac{1}{2} \sum_{\{i,j\} \in E_0} d_{ij}^{(0)} \left(X_i X_j + Y_i Y_j \right), \qquad (8)$$

where X, Y and Z are the standard Pauli matrices and d_{ij} are real-valued coupling constants. The Hamiltonians are therefore given by real-symmetric matrices.

We can similarly add control to the network by modifying a subset of the couplings defined by the edge set of a second graph, $G_C = (V_0, E_C)$

$$H_C := \frac{1}{2} \sum_{\{i,j\} \in E_C} d_{ij}^C \left(X_i X_j + Y_i Y_j \right), \qquad (9)$$

The controlled coupling can be manipulated either by a simple on-off sequence or more complicated pulses. It can easily be shown that the system Hamiltonian commutes with the total spin operator: $[H_0, S_Z] = 0$ for $S_Z := \sum_{i=1}^{N} Z_i$ and thus the number of excitations in the system is preserved, i.e., the dynamic Lie algebra is a direct sum of N subalgebras, each corresponding to the evolution of $k \in \{1, \dots, N\}$ excitations along the chain. The control H_C also preserves the coupling isotropy in the xy-plane and thus also commutes with the total spin operator, $[H_C, S_Z] = 0$, preserving the decomposition into excitation subspaces. The system is therefore not controllable in a conventional sense and would be unsuitable for N-qubit quantum computation without the addition of some control that does not commute with S_Z in order to break this symmetry and couple the sub-blocks of the Hamiltonian. However, for information transfer and state manipulations, excitation preservation is a positive property to exploit, automatically confining the dispersion of the excitation(s) within a lower-dimensional subspace. This will allow us to show how a single excitation can be forced to propagate to a chosen target state of the network.

Within the first excitation subspace, we use the basis $|n\rangle$ to denote an excitation localized on the nth qubit. Similarly, in the second excitation subspace we use $|n, m\rangle$ to denote a pair of excitations on qubits n and m. In a slight abuse of this notation, given a state $|\psi\rangle = \sum_{n=2}^{N} \alpha_n |n\rangle$, we will write $|1, \psi\rangle$ to denote $\sum_{n=2}^{N} \alpha_n |1, n\rangle$.

We shall use the matrices A and C to denote the restriction of H_0 and H_C to the single excitation subspace. A is an $N \times N$ matrix with elements $d_{ij}^{(0)} \neq 0$ for any pair

(i, j) which constitutes an edge of the underlying graph (and similarly for C using d_{ij}^C instead). For simplicity, we shall take $d_{ij}^{(0)} > 0$. If all $d_{ij}^{(0)} = 1$, then A corresponds to the adjacency matrix of the graph G_0. Note that all diagonal elements of both matrices are zero.

Although the following analysis could be conducted for more general controlling interactions, in the spirit of analyzing the capabilities of systems with minimalistic control, we consider controlling interactions of *pendant* type, i.e. in graph G_0, vertex 1 is unconnected (meaning $A_{1j} = A_{j1} = 0$ for all j), whereas the only edge in G_C is between vertices 1 and 2. Without loss of generality, we can take $d_{12}^C = 1$, corresponding to a control Hamiltonian

$$H_C := \frac{1}{2} \left(X_1 X_2 + Y_1 Y_2 \right). \qquad (10)$$

In the first instance, we assume that the coupling strengths are all known.

We first prepare the network in the zero-excitation state using a suitably strong background magnetic field [33], and initialize a state transfer or a single excitation state preparation task by introducing a single excitation on the pendant qubit. Given the initial state $|1\rangle$ on the pendant qubit and a target state $|\psi\rangle$ in the single excitation subspace, what is the optimal fidelity that can be achieved through modulation of the control C?

We start by applying the symmetry conditions to the particular case of a pendant controlled spin network, restricted to the first excitation subspace. Let M be a symmetry operator of the system. Then

$$MA \pm AM = 0,$$
$$MC \pm CM = 0,$$

where the sign determines whether the symmetry is of ASO or CSO type and must take the same value for both equations.

If M is a CSO, then $|1\rangle$ must be an eigenstate of M. Also, the eigenvectors of C, $|1\rangle \pm |2\rangle$ must be eigenstates of M. Combining these statements, $|2\rangle$ is an eigenstate of M, and this is in the same eigenspace as $|1\rangle$. Any eigenstate of A that is in a different eigenspace of M must satisfy $\langle 1|C|\lambda\rangle = 0$, and cannot be accessed. This allows us to show that degeneracies of the system are necessarily associated with symmetries. If A has degenerate eigenvalues then we have an eigendecomposition $A = \sum_k \lambda_k \Pi_k$, where Π_k are projectors onto the respective eigenspaces, and we have either $\Pi_k |2\rangle = 0$, in which case there is no overlap of state $|2\rangle = C|1\rangle$ with the kth eigenspace, or we can define an eigenbasis such that $|\lambda_{k,1}\rangle = \Pi_k |2\rangle$. As the projection of a vector onto a subspace cannot have more than rank 1, all other eigenvectors $|\lambda_{k,\ell}\rangle$ in the kth eigenspace must have zero overlap with state $|2\rangle$, and thus each $|\lambda_{k,\ell}\rangle\langle\lambda_{k,\ell}|$ for $l > 1$ commutes with both A and C and is therefore a CSO. This means that when we work under the assumption of having found all CSOs, we can take the subspaces to be

non-degenerate. Henceforth, we shall use $\mathcal{H}_a$ to denote the smallest subspace with support on $|2\rangle$, i.e. the space that remains relevant for tasks state manipulation tasks where we start in the state $|1\rangle$ when we remove all the CSOs from the single excitation subspace. Now we wish to identify the ASOs on $\mathcal{H}_a$, as these are the only ones that could affect our state manipulation task, potentially reducing the achievable fidelity below that of Eqn. (6).

Theorem 1. *In a pendant-controlled system with the pendant qubit indexed as qubit 1, if G_0 is a graph which is connected on vertices 2 to N with positive weights, $d_{ij}^{(0)} > 0$, a necessary and sufficient condition for the existence of an ASO that applies to $\mathcal{H}_a$ is that G_0 is bipartite (two-colorable).*

Proof. We start by noting that if G is bipartite, we can easily give an ASO within the single excitation subspace. For a graph to be bipartite, it means that we can partition the vertices into two sets $\{V_A, V_B\}$ such that edges only connect between the sets, not within a set. If we apply a product of Z operations on one side of that bipartition, then every $(XX + YY)$ coupling is affected by exactly one Z operator, with which it anticommutes. Hence, this is an ASO, and applies in all excitation subspaces.

In case there are additional CSOs that apply within the single excitation subspace, we need to justify that this ASO will also apply to just $\mathcal{H}_a$. Let M be the matrix representing the ASO in the single excitation subspace. We can write it as the diagonal matrix

$$M = \sum_{n \in V_A} |n\rangle\langle n| - \sum_{n \in V_B} |n\rangle\langle n|.$$

As with all ASOs, M imposes that the eigenvectors of A, $|\lambda_n\rangle$ either have 0 eigenvalue or arise in $\pm\lambda_n$ pairs with the eigenvector of eigenvalue $-\lambda_n$ being given by $M|\lambda_n\rangle$. This is proven by using the anticommutation,

$$A(M|\lambda_n\rangle) = -MA|\lambda_n\rangle = -\lambda_n(M|\lambda_n\rangle).$$

Now let's imagine there's another CSO that applies to both A and C. Thus, there must be a unitary matrix that acts on A and C to create the subspace structure. This additional structure is composed of eigenvectors $|\lambda_n\rangle$ of A with $\langle 2|\lambda_n\rangle = 0$. If these eigenvectors are subject to the ASO M, then the remaining subspace must also be subject to it. If $\langle 2|\lambda_n\rangle = 0$, then is also holds that $\langle 2|M|\lambda_n\rangle = 0$, so for any $\lambda_n \neq 1$, eigenvectors can be removed in pairs. These pairs manifest within A or C as a subspace

$$S = |\lambda_n\rangle\langle\lambda_n| - M|\lambda_n\rangle\langle\lambda_n|M^\dagger.$$

Since $M^2 = \mathbf{1}$, we have that

$$\{S, M\} = 0.$$

On the other hand, if $\lambda_n = 0$, then we just have $S = 0$, and thus $\{S, M\} = 0$ So, for each subspace that we remove, the matrix M splits into two components, an ASO for the removed subspace, and an ASO for the remaining one.

If M were to remain diagonal under the action of that unitary, then M would also have the same subspace structure, and we could just extract that $\mathcal{H}_a$ component. If we are removing an eigenvector $|\lambda_n\rangle$ from the space, then it is because it has $\langle 2|\lambda_n\rangle = 0$, which will also be true for the eigenvector $M|\lambda_n\rangle$ i.e. for non-zero eigenvalues, the eigenvectors must be removed in pairs.

Moreover, it is the only relevant ASO in the single excitation subspace.

Lemma 1. *Having taken into account all CSOs, $\mathcal{H}_a$ for a pendant-controlled system has no more than one ASO.*

Proof. We can take the restriction of C to $\mathcal{H}_a$ to be $C = |1\rangle\langle 2| + |2\rangle\langle 1|$, and the restriction of A to $\mathcal{H}_a$ is A', which has N_a eigenvectors $|\lambda_n\rangle$. We can always take that $|\lambda_1\rangle = |1\rangle$, which is a 0 value eigenvector of A'.

Assume there exists an M which anticommutes with both C and A'. Anticommutation with C means the structure of M must be such that $|1\rangle$ and $|2\rangle$ are eigenvectors with eigenvalues of equal magnitude but opposite sign. We can fix the scale factor of the matrix by specifying that $|2\rangle$ is the $+1$ eigenvalue. Anticommutation with A' implies that eigenvectors come in $\pm\lambda_n$ pairs, with a single 0 eigenvector if N_a is even. We order the eigenvectors such that the eigenvalues $\lambda_n = -\lambda_{n+n_a}$ for $n = 2$ to $1 + n_a$ with $n_a = \lfloor (N_a - 1)/2 \rfloor$. Hence, we can write M as

$$M = -|1\rangle\langle 1| + \sum_{n=2}^{1+n_a} \beta_n(|\lambda_n\rangle\langle-\lambda_n| + |-\lambda_n\rangle\langle\lambda_n|). \quad (11)$$

If N_a is even then A' has a second 0-eigenvalue ($|\lambda_{N_a}\rangle$) which adds a term $\beta_{N_a}|\lambda_{N_a}\rangle\langle\lambda_{N_a}|$ to M. Let $U = \sum_{n=1}^{N_a} |n\rangle\langle\lambda_n|$ be the unitary operator that diagonalizes A'. Then $UA'U^\dagger =$

$$\begin{cases} \text{diag}(0, \lambda_2, \lambda_3 \ldots \lambda_{1+n_a}, -\lambda_2, -\lambda_3 \ldots) & N_a \text{ odd} \\ \text{diag}(0, \lambda_2, \lambda_3 \ldots \lambda_{1+n_a}, -\lambda_2, -\lambda_3 \ldots, 0) & N_a \text{ even.} \end{cases}$$

The action of U also simplifies M, $UMU^\dagger =$

$$\begin{cases} (-1) \oplus (X \otimes \text{diag}(\beta_2, \beta_3 \ldots \beta_{1+n_a})) & N_a \text{ odd} \\ (-1) \oplus (X \otimes \text{diag}(\beta_2, \beta_3 \ldots \beta_{1+n_a})) \oplus \beta_{N_a} & N_a \text{ even.} \end{cases}$$

As $|2\rangle$ is a $+1$ eigenvector, we have $M|2\rangle = |2\rangle$. Defining

$$|v\rangle = \begin{cases} (1 \oplus (H \otimes \mathbf{1})) U^\dagger|2\rangle & N_a \text{ odd} \\ (1 \oplus (H \otimes \mathbf{1}) \oplus 1) U^\dagger|2\rangle & N_a \text{ even} \end{cases}$$

where H is the Hadamard gate, it follows that $|v\rangle$ is a $+1$ eigenvector of $(H \otimes \mathbf{1})M(H \otimes \mathbf{1})$, which is a diagonal matrix. Evidently, one of $\langle n|v\rangle$ and $\langle n + n_a|v\rangle$ must be 0 for $n \geq 2$. However, both cannot be 0 because that would imply $\langle n|v\rangle \pm \langle n + n_a|v\rangle = 0$, and thus $\langle n|U^\dagger|2\rangle = \langle\lambda_n|2\rangle = 0$, which is not allowed since there are no CSOs on $\mathcal{H}_a$. This uniquely determines M. If N_a is even, the remaining coefficient $\beta_{N_a} = 1$ as we must have $\langle N_a|v\rangle = \langle\lambda_{N_a}|2\rangle \neq 0$. $\square$

It remains to prove that non-bipartite graphs do not have an ASO on $\mathcal{H}_a$. Let us assume the contrary – there exists an ASO, M. This means that all the eigenvectors $|\lambda_n\rangle$ with eigenvalue $\lambda_n \neq 0$ have a counterpart $M|\lambda_n\rangle = |-\lambda_n\rangle$ of eigenvalue $-\lambda_n$. Moreover, as argued above, $|2\rangle$ is an eigenvector of the symmetry operator, so these eigenvectors have the same value of $\alpha_n := \langle 2|\lambda_n\rangle$. Following a similar route to [2], this assumption imposes that

$$\langle 2|A^{2k+1}|2\rangle = \sum_n |\alpha_n|^2 \lambda_n^{2k+1} = 0. \qquad (12)$$

We can also expand the $\langle 2|A^{2k+1}|2\rangle$ in terms of the coupling strengths $d_{ij}^{(0)}$; it is a sum of paths of $2k+1$ steps starting and ending on vertex 2, where for each path we just take the product of the coupling strengths along that path. The existence of such a path implies the existence of an odd cycle in the graph i.e. for bipartite graphs, $\langle 2|A^{2k+1}|2\rangle = 0$. For a non-bipartite graph, however, there do exist odd loops. If all the $d_{ij}^{(0)} > 0$, then the product around any given path is positive, and the sum over all paths must also be positive i.e. there must exist a k for which $\langle 2|A^{2k+1}|2\rangle > 0$, and we must see such a path if the graph is connected and all the coupling strengths are positive; Eqn. (12) must be violated, and there cannot be an ASO[34]. Whether we operate in the single excitation subspace or $\mathcal{H}_a$ does not matter to this argument as the only difference is the presence or absence of eigenvectors with $\alpha_n = 0$, which therefore do not affect $\langle 2|A^{2k+1}|2\rangle$. $\qquad\square$

Theorem 2 (Maximum transfer fidelity). *Let A correspond to the single excitation subspace of an XX Hamiltonian with positive weights, and a coupling geometry specified by a graph G_0 that is connected and not bipartite. In conjunction with a pendant-type control C, the maximum fidelity for transfer of an initial state $|1\rangle$ to a target state $|\psi\rangle$ in the single-excitation subspace is*

$$F_{1\mapsto\psi} = 1 - \sum_{\{(k,\ell)|\langle 1|C|\lambda_{k,\ell}\rangle=0\}} |\langle\psi|\lambda_{k,\ell}\rangle|^2, \qquad (13)$$

and this bound is attainable, provided $\{|\lambda_{k,\ell}\rangle\}$ is an eigenbasis of A with $\ell = 1, \ldots, rank(\Pi_k)$ satisfying

$$\langle 1|C|\lambda_{k,\ell}\rangle = 0, \qquad \forall k, \ \forall \ell > 1, \ and \qquad (14a)$$
$$\Pi_m|\lambda_{k,\ell}\rangle = 0, \qquad \forall m \neq k \qquad (14b)$$

where Π_k is the projector onto the k-th eigenspace.

Proof. Let us assume that A has an eigendecomposition

$$A = \sum_n \lambda_n |\lambda_n\rangle\langle\lambda_n|.$$

We can always take $|\lambda_1\rangle = |1\rangle$ and $\lambda_1 = 0$ as $|1\rangle$ is an eigenstate of A with eigenvalue 0. Moreover, by the definition of the pendant-type control system the only

connection of this subsystem to the rest of the network is through state $|2\rangle$ via C. Define the C-overlaps

$$\alpha_n := \langle 1|C|\lambda_n\rangle = \langle 2|\lambda_n\rangle, \qquad (15)$$

and let $I_0 = \{n|\alpha_n \neq 0\}$. If $\alpha_n = 0$ then the subspace spanned by $|\lambda_n\rangle$ is decoupled and cannot be accessed. Hence, any state produced from the initial state using the control must be a superposition of eigenstates $|\lambda_n\rangle$ that have non-zero overlap with $|2\rangle$,

$$|\phi\rangle = \sum_{n\in I_0} \gamma_n|\lambda_n\rangle.$$

Writing the target state $|\psi\rangle$ in the A-eigenbasis $|\psi\rangle = \sum_n \beta_n^{(\psi)}|\lambda_n\rangle$, the overlap of the output state with $|\psi\rangle$ is

$$F_{1\mapsto\psi} = |\langle\phi|\psi\rangle|^2 = \left|\sum_{n\in I_0} \gamma_n^* \beta_n^{(\psi)}\right|^2.$$

As we must have $\sum_n |\gamma_n|^2 = 1$ and $\gamma_n = 0$ for $n \notin I_0$, the overlap is maximised if we choose

$$\gamma_n = \frac{\beta_n^{(\psi)}}{\sqrt{\sum_{n\in I_0} |\beta_m^{(\psi)}|^2}}, \qquad \forall n \in I_0.$$

in which case we obtain

$$F_{1\mapsto\psi} = \left|\frac{\sum_{n\in I_0} |\beta_n^{(\psi)}|^2}{\sqrt{\sum_{n\in I_0} |\beta_n^{(\psi)}|^2}}\right|^2 = \sum_{n\in I_0} |\beta_n^{(\psi)}|^2$$
$$= 1 - \sum_{n\notin I_0} |\beta_n^{(\psi)}|^2 = 1 - \sum_{n\notin I_0} |\langle\psi|\lambda_n\rangle|^2.$$

A non-bipartite graph has no ASOs, so we have frequency-selective control of each transition $|1\rangle \mapsto |\lambda_n\rangle$ for which the transition probability $|\langle\lambda_1|C|\lambda_n\rangle|^2$ does not vanish by using a Rabi oscillation of the control field C with frequency $\omega_{1n} = \lambda_n - \lambda_1 = \lambda_n$. There are some special cases which we have to handle. It can be the case that there are two eigenvectors with eigenvalue $\pm\lambda$. Provided that the $|\alpha_n|$ are distinct, a Rabi oscillation still suffices via judicious choice of pulse timing. If the $|\alpha_n|$ are also equal, one has to use a different technique – we find a different level $|\kappa\rangle$ which we populate first, and then perform a two frequency (Raman) transition with frequencies $\lambda - \Delta$ and $\kappa - \Delta$, where Δ is a detuning. The only way that this technique can fail is if the system is so structured that all eigenvectors satisfy this pairing property, or have 0 eigenvalue i.e. there is an ASO present, but we know there is no such ASO.

We can therefore, in principle, transform the state $|1\rangle$ to the output state $|\phi\rangle$ by applying a sequence of pulses resonant with the transition frequencies λ_n as in [5], for instance. With arbitrarily slow and weak pulses, the off-resonant excitations are arbitrarily weak, however off-resonant excitations could be suppressed, transfer times

reduced, and other constraints introduced, by using optimal control pulse design [9, 19]. In the case of an on-off control switch, we could try to match the frequencies in the Fourier decomposition of the square pulses with the resonant frequencies as pointed out in [5]. □

In the case of bipartite graphs, there is an ASO present, and attempting a Rabi oscillation using C to address the transition between $|1\rangle$ and $|\lambda_n\rangle$ equally couples to the transition between $|1\rangle$ and $|-\lambda_n\rangle$, so we can only prepare paired eigenvectors in states

$$e^{i\lambda_n t}|\lambda_n\rangle + e^{-i\lambda_n t}|-\lambda_n\rangle$$

i.e. they have the same mod-square amplitude. In a similar way to Example 1, we will prove that this happens however we attempt to control the system, and give a physical interpretation of the states satisfying this property.

Lemma 2. *A state transformation task on a bipartite pendant controlled graph can be implemented up to the bounds specified in Theorem 2 if and only if the target state has (up to a global phase) real amplitudes on one of the bipartitions, V_A and imaginary amplitudes on the other, V_B.*

Proof. The states that we can make are of the form

$$|\psi_{\text{targ}}\rangle = \sum_n \beta_n (e^{i\phi_n}|\lambda_n\rangle + e^{-i\phi_n}|-\lambda_n\rangle)$$

with real β_n. The bipartite graph in the subspace $\mathcal{H}_a$ (any weight of the target state outside this space is explicitly forbidden by Theorem 2) has exactly one ASO. It suffices for us to describe its effect on the single excitation subspace since we have already seen how this symmetry splits under the action of any further CSOs.

$$M = \sum_{n \in V_A} |n\rangle\langle n| - \sum_{n \in V_B} |n\rangle\langle n|.$$

Since all eigenvectors $|\lambda_n\rangle$ of A have $M|\lambda_n\rangle = |-\lambda_n\rangle$, $|\lambda_n\rangle$ and $|-\lambda_n\rangle$ have real amplitudes γ_{nm} with equal modulus on every spin m, and the relative phase in amplitude, ± 1, is determined entirely by which side of the bipartition they sit on. Hence,

$$|\psi_{\text{targ}}\rangle = 2 \sum_{m \in V_A} \sum_n \beta_n \gamma_{nm} \cos(\phi_n)|m\rangle$$
$$+ 2i \sum_{m \in V_B} \sum_n \beta_n \gamma_{nm} \sin(\phi_n)|m\rangle.$$

All the amplitudes on V_A are real, all those on V_B are imaginary and all such amplitudes are reachable.

To see that the transformation is otherwise impossible, consider the operator
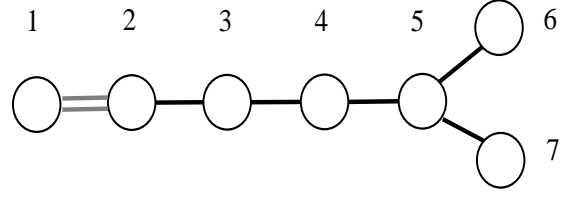
$$U_B = \prod_{n \in V_B} \sqrt{Z_n}.$$

FIG. 1: Controlled interaction between spins 1 and 2 marked double in gray

If we transform H_0 and H_C according to U_B, all $(XX + YY)$ terms are transformed into $(XY - YX)$ terms, which are imaginary. Hence, all evolutions $-iU_B(H_0 + f(t)H_C)U_B^\dagger$ are real, and the corresponding unitary operators are real. By starting with a state $U_B|1\rangle = |1\rangle$, which is real, the amplitudes of all output states $U_B|\psi\rangle$ must be real. Thus $|\psi\rangle$ must be real on spins that are in V_A, and imaginary on those in V_B. □

In particular, this means that state transfer tasks are unaffected by ASOs. The phase result makes a lot of sense because we know that evolution under a Hamiltonian $\frac{1}{2}(XX + YY)$ leads to a hopping term between two vertices, but introduces a phase factor of $-i$ for each hop. Hence, on a bipartite graph, if we start on a single site with a real amplitude, all those that are an even number of hops away (which is only well defined on a bipartite graph) must have a real amplitude, whereas those that are an odd number of hops away must have an imaginary amplitude.

Alternatively, the limitation is easily overcome – we can introduce a second control field $C' = i|1\rangle\langle 2| - i|2\rangle\langle 1|$, which corresponds to a coupling $\frac{1}{2}(X_1Y_2 - Y_1X_2)$. As this coupling is not real, it does not satisfy (3), although it does still anticommute with the symmetry operator. Using a Rabi oscillation of $\cos(\omega_{1n}t)C \pm \sin(\omega_{1n}t)C'$ allows us to selectively make the transition of one or other of the eigenvectors. This illustrates the important difference between the symmetry condition of Eqn. (3) and anticommutation if the Hamiltonian is not real-valued. With this additional control in place, the conditions of Thm. 2 are all achievable. However, we will not further consider this control.

In summary, we see that in all cases the maximum possible state transfer fidelity is entirely determined by the energy eigenstates of A which have zero overlap with $|2\rangle$, the point where the pendant control meets the rest of the system. Entanglement generation, however, is additionally affected in bipartite graphs by whether the pair of qubits that are to be entangled are separated by an even or odd number of edges, and the relative phase to be generated between the pair – we can either make $|n\rangle + |m\rangle$ for even distances, or $|n\rangle + i|m\rangle$ for odd distances.

Example 2: First we examine a uniformly XX-coupled N-spin chain with a fork at the end (see Fig. 1), initialized with a single excitation localized on the first qubit. Diagonalizing the adjacency matrix shows that the only
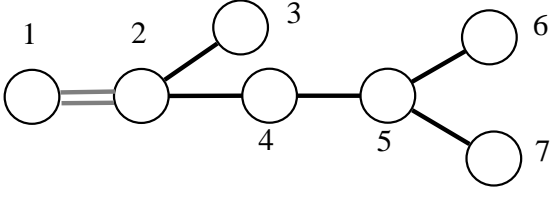
FIG. 2: Controlled interaction between spins 1 and 2 marked double in gray

eigenstate with zero C-overlap is $|\lambda_-\rangle = \frac{1}{\sqrt{2}}(|6\rangle - |7\rangle)$. Consider state transfer to $|6\rangle$; when we write this in the adjacency matrix eigenbasis, the coefficient of the $|\lambda_-\rangle$ eigenstate is $\beta_-^{(6)} = 1/\sqrt{2}$, giving a maximum transfer fidelity $F_{1\mapsto6} = 1 - |\beta_-^{(6)}|^2 = 1 - |\frac{1}{\sqrt{2}}|^2 = \frac{1}{2}$; the same result is obtained for transfer to $|7\rangle$ by symmetry. This is to be expected; the two end qubits are in some sense indistinguishable, and we cannot direct information flow to either one specifically. At all times, the control addresses both simultaneously, and so we obtain a superposition state over these two qubits. This is made clear in the algorithmic computations. In this case, the Hamiltonian is symmetric under the change of basis CSO J_{67} taking $J_{67}|6\rangle = |7\rangle$, $J_{67}|7\rangle = |6\rangle$, $J_{67}|n\rangle = |n\rangle$ otherwise. Performing the computations above shows that the Hamiltonian in this subspace generates a dynamical Lie algebra of $\mathfrak{so}(6) \oplus \mathbf{1}$, where the $\mathbf{1}$-term corresponds to the subspace spanned by the dark state $\frac{1}{\sqrt{2}}(|6\rangle - |7\rangle)$. If our initial state has no overlap with this state then it remains unpopulated and "dark" throughout. Alternatively if our initial state is contained in this subspace, it will be preserved throughout the system's evolution. On the other hand, we can choose to produce states such as $(|6\rangle+|7\rangle)/\sqrt{2}$, which is an entangled state, or states such as $|5\rangle$, which would allow perfect transfer of an unknown qubit state from qubit 1 to qubit 5. However, without the additional control C', it is impossible to perfectly produce states such as $\frac{1}{\sqrt{2}}(|3\rangle + |4\rangle)$ as a result of the bipartite nature of the graph, and the disruption caused by the ASO.

The results in the previous example are intuitive, but, for other systems, identifying the symmetries and dark subspaces may be less intuitive.

Example 3: If we make a small modification to the system in Fig. 1 by moving the pendant vertex as shown in Fig. 2, then additional symmetries and dark states arise. Since the graph is bipartite, with partitions $V_1 = \{1,3,4,6,7\}$ and $V_2 = \{2,5\}$, we can immediately observe that there is an ASO

$$M = \mathbf{1} - 2(|2\rangle\langle2| + |5\rangle\langle5|),$$

derived from $Z_2 Z_5$, which anticommutes with the Hamiltonian. We again observe the permutation CSO

$$J_{67} = \mathbf{1} - (|6\rangle - |7\rangle)(\langle6| - \langle7|),$$

which commutes with the Hamiltonian. These two symmetry operators give rise to an eigenspace of eigenvalue zero which has no overlap with $|2\rangle$ and is spanned by the vectors

$$|\lambda_{0,1}\rangle = \frac{1}{\sqrt{2}}(|6\rangle - |7\rangle),$$

$$|\lambda_{0,2}\rangle = \frac{1}{\sqrt{10}}(2|3\rangle - 2|4\rangle + |6\rangle + |7\rangle).$$

No other eigenvectors have zero overlap with $|2\rangle$ thus the maximum transfer fidelity to $|3\rangle$, for example, is $F_{1\mapsto3} = 1 - |\beta_1^{(3)}|^2 - |\beta_2^{(3)}|^2 = \frac{3}{5}$ as $\beta_1^{(3)} = 0$ and $\beta_2^{(3)} = \frac{2}{\sqrt{10}}$. Similarly, the state $\frac{1}{\sqrt{2}}(|6\rangle + |7\rangle)$ can only be produced with fidelity $1 - \frac{1}{5} = \frac{4}{5}$.

IV. CATALYTIC EXCITATIONS AND THE CLASSIFICATION OF DARK STATES

So far we have discussed access to states in the first-excitation subspace using paths entirely within this subspace, as assumed universally in prior works. The controlling interaction was assumed to commute with the total spin operator S_Z and was thus unable to produce paths which move between excitation subspaces. To access dark states, we could modify the control so that it does not commute with S_Z, breaking the symmetry and thus the excitation subspace structure. Doing so could lead to difficulties: the resulting subspaces will be of much larger dimension, and this will increase the computational difficulty of finding controls. The higher dimensional systems are more likely to contain uncharacterized resonances which makes it harder to produce controls which confine the excitations to the desired path in state space. However, we shall now show that moving to higher excitation subspaces can sometimes be advantageous and need not complicate the control too much.

In general, breaking symmetries requires changing the control Hamiltonians or adding new controls. However, in some cases we can avoid certain symmetries by moving to higher excitation subspaces, using our ability to introduce additional excitations on the first spin, which has been implicitly present as a control within the initialization stage, but we have not explicitly considered it when deriving accessible states. To produce a desired target state $|f_k\rangle$ in the k-excitation subspace, we may be able to bypass symmetry-induced restrictions in this subspace by temporarily introducing additional excitations, which we shall call *catalytic* excitations. To do so, we pass to the l-excitation subspace which contains a state of the form $|f_k\rangle \otimes |\phi\rangle$ in its reachable set, and finally extract the excess excitations to leave $|f_k\rangle$. Not all symmetries can be avoided this way; permutation symmetries which do not act on qubit 2 certainly cannot be avoided. However, in many cases, adding a single extra excitation will suffice.

From [20], we have

Definition. *The matrix representing the second excitation subspace of H_0 is given by*

$$\Lambda^2(A)_{mn} :=$$
$$\frac{1}{4}|(\langle k,l| - \langle l,k|)\,[I_N \otimes A + A \otimes I_N]\,(|i,j\rangle - |j,i\rangle)| \quad (16)$$

for $m := (N-1)k + l$ and $n := (N-1)i + j$, where $|i,j\rangle$ denotes the vertices at which the excitations are localized.

Similarly, $\Lambda^2(C)$ is the action of the control upon this subspace. The connectedness of this graph under basis changes (and thus the irreducibility of the dynamical Lie algebra) is not easily determined from the connectedness of A and C [35]. In other words, the existence, or lack thereof, of ASOs and CSOs other than permutation symmetries in one excitation subspace does not necessarily imply their existence in another excitation subspace, therefore we must search for them in each subspace separately. It is this feature that potentially enables catalysis, illustrating that, in general, it is not sufficient for analyses of state transfer in spin networks to restrict to the single excitation subspace.

Theorem 3 (Sufficient condition for increased control through catalytic excitations)**.** *A system has an accessible pair $(|\psi_{in}\rangle, |\psi_{out}\rangle)$ in the single excitation subspace using catalytic excitations (assuming $\langle 1|\psi_{out}\rangle = 0$) if it has accessible pairs $(|\psi_{in}\rangle, |\psi'\rangle)$ and $(|1, \psi'\rangle, |1, \psi_{out}\rangle)$ with $\langle 1|\psi'\rangle = 0$.*

Proof. Initialize the system in the state $|1\rangle$ and transform it to the state $|\psi'\rangle$ in the single-excitation subspace, which by hypothesis is accessible and satisfies $\langle 1|\psi'\rangle = 0$. Introducing a second *catalytic* excitation at the first site then produces the state $|1\rangle \otimes |\psi'\rangle$ in the second excitation subspace, and by hypothesis, we can create the state $|1\rangle \otimes |\psi_{out}\rangle$. Removing the catalytic excitation on the first site, we are left with our desired target state, $|\psi_{out}\rangle$. $\square$

We now give an example to prove that such a situation can arise, even when $(|\psi_{in}\rangle, |\psi_{out}\rangle)$ are not an accessible pair when confined to evolution solely within the single excitation subspace.

Example 4: For the system given in Fig. 2, we saw in Example 3 that the target state $|3\rangle$ is not perfectly accessible from the initial state $|1\rangle$. As before, we look at the eigenbasis of A where we have eigenvectors corresponding to eigenvalues of $\lambda_0 = 0$ and $\lambda_{\pm,\pm} = \pm\sqrt{(5 \pm \sqrt{5})/2}$. Labelling the corresponding eigenvectors $|\lambda_0\rangle$ and $|\lambda_{++}\rangle$, $|\lambda_{-+}\rangle$, etc. we have

$$|3\rangle = \sqrt{\frac{2}{5}}|0\rangle + \frac{\sqrt{10}-\sqrt{2}}{4\sqrt{5}}(|\lambda_{++}\rangle + |\lambda_{-+}\rangle)$$
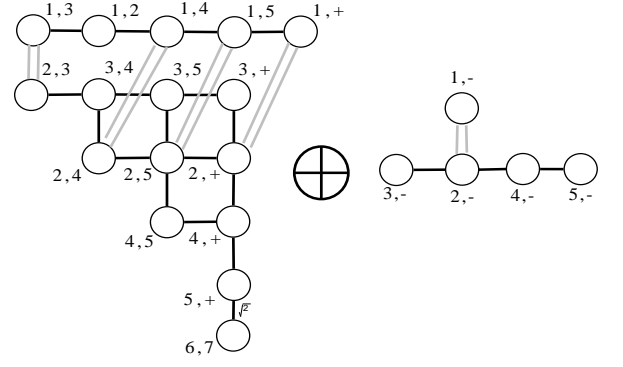$$+ \frac{\sqrt{10}+\sqrt{2}}{4\sqrt{5}}(|\lambda_{+-}\rangle + |\lambda_{--}\rangle)$$

FIG. 3: Controlled interactions marked double in gray; i,j represents product state $|i\rangle|j\rangle$; + represents $\frac{1}{\sqrt{2}}(|6\rangle + |7\rangle)$, - represents $\frac{1}{\sqrt{2}}(|6\rangle - |7\rangle)$. Note that the controlled couplings are simultaneously controlled, not independently.

and starting from $\alpha|0\rangle + \beta|1\rangle$, the state with maximum overlap with $|3\rangle$ we can achieve is

$$\alpha|0\rangle + \beta\left[\frac{|3\rangle - \sqrt{\frac{2}{5}}(\sqrt{\frac{2}{5}}|3\rangle - \sqrt{\frac{2}{5}}|4\rangle + \sqrt{\frac{1}{10}}(|6\rangle + |7\rangle))}{\sqrt{\frac{3}{5}}}\right]$$

with maximum fidelity [36]

$$\sqrt{F_{(\alpha|0\rangle+\beta|1\rangle)\mapsto(\alpha|0\rangle+\beta|3\rangle)}} = |\alpha|^2 + |\beta|^2\sqrt{\frac{3}{5}}.$$

Instead of this, we could first produce

$$\alpha|0\rangle + \beta\Big[\frac{\sqrt{10}+\sqrt{2}}{4\sqrt{5}}(|\lambda_{+-}\rangle + |\lambda_{--}\rangle)$$
$$+ \sqrt{\frac{1}{10}(7 - \sqrt{5})}(|\lambda_{++}\rangle + |\lambda_{-+}\rangle)\Big],$$

defining $|\psi'\rangle$, and then introduce a single *catalyst excitation* at spin 1,

$$\alpha|1\rangle + \beta\Big[\frac{\sqrt{10}+\sqrt{2}}{4\sqrt{5}}(|1, \lambda_{+-}\rangle + |1, \lambda_{--}\rangle)$$
$$+ \sqrt{\frac{1}{10}(7 - \sqrt{5})}(|1, \lambda_{++}\rangle + |1, \lambda_{-+}\rangle)\Big].$$

We have moved into a superposition of the 1 and 2-excitation subspaces, and our control will keep the state in these subspaces. To show that we can reach the target state using catalytic excitations we need to prove that the set of states

$$\{(|1, \psi'\rangle, |1, \psi_{out}\rangle), (|1\rangle, |1\rangle)\}$$

are simultaneously accessible such that the $|0\rangle$ component of the unknown state is also correctly transferred. This 2-excitation subspace has no dark states which are left uncoupled to the controlling interaction, except those

which are a product of $\frac{1}{\sqrt{2}}(|6\rangle - |7\rangle)$ and a single excitation on one of qubits 1 to 5. Examining the graph produced by the Hamiltonian for the 2-excitation subspace (Fig. 3, formed as in [20]), we can see that there are no eigenstates of the Hamiltonian for the left-hand component (i.e. the connected component to our initial state) that have no overlap with all the states our control connects to. This is the analogue to checking which states had $\langle 1|C|\lambda_n\rangle = 0$ above.

We select an eigenvector $|\tilde{\lambda}\rangle$ in the second excitation subspace. Based on this choice, we apply a field of $d_{12} \propto \cos((\lambda_{++} - \tilde{\lambda})t)$ on the controlled coupling between spins 1 and 2, and, neglecting off-resonant excitations, we obtain an effective coupling

$$H_1 \propto |1, \lambda_{++}\rangle\langle\tilde{\lambda}| + |\tilde{\lambda}\rangle\langle 1, \lambda_{++}|$$
$$+ |1, \lambda_{-+}\rangle\langle-\tilde{\lambda}| + |-\tilde{\lambda}\rangle\langle 1, \lambda_{-+}|$$

which can transform the state to

$$\alpha|1\rangle + \beta\Big[\frac{\sqrt{10}+\sqrt{2}}{4\sqrt{5}}(|1, \lambda_{+-}\rangle + |1, \lambda_{--}\rangle) + \sqrt{\frac{1}{5}}(|\tilde{\lambda}\rangle$$
$$+ |-\tilde{\lambda}\rangle) + \frac{\sqrt{10}-\sqrt{2}}{4\sqrt{5}}(|1, \lambda_{++}\rangle + |1, \lambda_{-+}\rangle)\Big].$$

Similarly, neglecting off-resonant excitations, applying a field $J_{12} \propto \cos(\tilde{\lambda}t)$ on the controlled transition gives rise to an effective Hamiltonian

$$H_2 \propto |1, \lambda_0\rangle\langle\tilde{\lambda}| + |\tilde{\lambda}\rangle\langle 1, \lambda_0| + |1, \lambda_0\rangle\langle-\tilde{\lambda}| + |-\tilde{\lambda}\rangle\langle 1, \lambda_0|$$

which can transform the previous state into

$$\alpha|1\rangle + \beta\Big[\frac{\sqrt{10}+\sqrt{2}}{4\sqrt{5}}(|1, \lambda_{+-}\rangle + |1, \lambda_{--}\rangle)$$
$$+ \sqrt{\frac{2}{5}}|1, \lambda_0\rangle + \frac{\sqrt{10}-\sqrt{2}}{4\sqrt{5}}(|1, \lambda_{++}\rangle + |1, \lambda_{-+}\rangle)\Big]$$
$$= \alpha|1\rangle + \beta|1, 3\rangle.$$

Removing the catalyst excitation from the first spin gives the desired final state, $\alpha|0\rangle + \beta|3\rangle$. Introducing this excitation allowed us to move between different subspaces induced by the symmetry.

Notice that the catalyst excitation cannot make the state $\frac{1}{\sqrt{2}}(|6\rangle - |7\rangle)$ accessible from an initial state $|1\rangle$ because the graph derived from the Hamiltonian will have two components, with one component comprising states of the form $|\psi\rangle \otimes \frac{1}{\sqrt{2}}(|6\rangle - |7\rangle)$ in all the excitation subspaces. Therefore, we can say that there are two types of dark state, one of which one is not as dark as the other. Dark states arising from a permutation of the qubits [17] are truly dark – they induce a splitting of the Hamiltonian which persists in all excitation subspaces, and which cannot be overcome without introducing a symmetry-breaking control. The second class of dark states are artifacts of the particular eigenvectors found in each subgraph, whose underlying symmetries may be

bypassed in higher excitation subspaces, potentially rendering them accessible. However, it should be noted that if A is a simple one-dimensional chain then these symmetries do persist, as can be proven via the Jordan-Wigner transformation [5].

V. SYSTEM IDENTIFICATION

Our control method in Sec. III, based on geometric control, is sub-optimal and, if the system Hamiltonian is known, there are various ways to derive control pulses that saturate the bounds. However, these require some basic knowledge of the Hamiltonian. In particular, given the promise of pendant control, we only need to know the eigenvalues λ_n, α_n (the overlaps of the eigenvector with $|2\rangle$, the single excitation on spin 2), and some information about the target state – its decomposition in terms of the eigenvectors. This decomposition must be specified with a particular phase convention for the eigenvectors, which we shall choose such that $\alpha_n > 0$ for all n. Numerical simulations further show that it is possible to derive pulses to achieve this threshold even when the Hamiltonian of the system has not been determined, using optimization over the record of multiple single-basis projective measurements on the target qubit, as developed in [9]. Indeed, we shall now prove that it is possible to identify the control parameters λ_n and α_n so that, if given a target state expressed in terms of the eigenvector decomposition, the state transformation task can be achieved without any further promises on the system.

For this, consider the same drift Hamiltonian A and control field C that we have used so far within the single excitation subspace. By determining the eigenvalues λ_n and overlaps $\alpha_n = \langle 2|\lambda_n\rangle$ of A', the restriction of A to the space $\mathcal{H}_a$, then if we are given a state transformation task starting from $|1\rangle$, with an output state described in terms of the amplitudes of different eigenvectors, we can implement that transformation optimally. Of course, in order to translate from a specification in terms of the spin basis will require further promises about the structure of A. To date [21, 22], such assumptions represent a massive restriction, so it is interesting to identify what aspect of the protocol it is that requires such assumptions.

Let us define

$$H = A + \varepsilon C,$$

and assume that H has eigenvectors $|\eta_n\rangle$. Our level of control can certainly allow us to measure, as a function of time, quantities such as

$$\left|\langle 1|e^{-iHt}|1\rangle\right|^2 = \left|\sum_n |\langle 1|\eta_n\rangle|^2 e^{-i\eta_n t}\right|^2,$$

a Fourier transform of which will reveal the eigenvalue differences $|\eta_n - \eta_m|$ and overlaps $|\langle 1|\eta_n\rangle|^2$. By assuming ε to be small, we can perform a perturbative expansion,

expressing these quantities in terms of the properties of A' that we wish to determine. In particular, for $n \neq 1$ and for $\lambda_n \neq 0$, we can write that, to first order, $\eta_n = \lambda_n$ and

$$|\eta_n\rangle = |\lambda_n\rangle + \frac{\varepsilon\langle 1|C|\lambda_n\rangle}{\lambda_n}|1\rangle,$$

i.e., $|\langle 1|\eta_n\rangle| = \varepsilon\alpha_n/\lambda_n$, so the α_n and $|\lambda_n - \lambda_m|$ are readily extracted for any eigenvector which does not have $\alpha_n = 0$ i.e. as one would expect, we cannot learn the properties of the states outside the space $\mathcal{H}_a$. If there is an eigenvector with $\lambda_m = 0$ and $\alpha_m \neq 0$, then we have to apply degenerate perturbation theory, but this just means the two 0 energy levels (including $|1\rangle$) mix, with energies $\pm\varepsilon\alpha_m$. Again, the relevant quantities can be extracted.

From the differences $|\lambda_n - \lambda_m|$, the eigenvalues can only be identified up to an overall global shift, λ_1, and the difference between $\lambda_n - \lambda_1$ and $-(\lambda_n - \lambda_1)$ cannot be distinguished. The global shift only alters the global phase in the subsequent state transformation protocol, and is therefore largely irrelevant, but we can still argue how to determine both of these features. Firstly, observe that neither affect a system with an ASO – we know that $H = -H$. Hence, we only have to deal with the case where the levels can, in principle, be addressed. For a given eigenvector $|\lambda_n\rangle$, we know α_n, but not the eigenvalue. By determining two such values, all ambiguity can be removed. If we have an eigenvector $|\lambda_n\rangle$ with eigenvalue λ_n, then provided there is not also an eigenvector with $-\lambda_n$ (if there is, we can adapt for it), we can perform a Rabi oscillation of C with frequency λ_n, and in some fixed time, as specified by $|\alpha_n|^2$, we return to our initial state, having gone down to a probability of $|\alpha_n|^2$ of being found in the state $|1\rangle$ half way through the protocol. Hence, for a unique value of $|\alpha_n|^2$, we can scan through all possible frequencies and find the relevant value of $|\lambda_n|$. In order to discover the sign of this energy (since a Rabi oscillation addresses $\pm\lambda_n$ simultaneously), we instead prepare $|0\rangle + e^{i\phi}|1\rangle$ for various values of ϕ, and transform it to $|0\rangle + e^{i\phi}|\lambda_n\rangle$, leave it for some time t so that it evolves to $|0\rangle + e^{i(\phi+\lambda_n t)}|\lambda_n\rangle$, and then return it to the initial state $|0\rangle + e^{i(\phi+\lambda_n t)}|1\rangle$. By measuring the probability $p = \cos^2(\frac{1}{2}(\phi + \lambda_n t))$ of getting the $|+\rangle$ measurement result, then provided $|\lambda_n|t \leq \pi$, the sign of

$$-\left.\frac{dp}{d\phi}\right|_{\phi=0}$$

is the same as that of λ_n.

This analysis reveals that within a pendant controlled system, it is, in principle, possible to extract the values λ_n and α_n that we need to know, although in practice one would undoubtedly develop more sophisticated protocols which do not rely on measuring extremely small quantities. Consequently, we observe that to implement a complete identification protocol such that we can produce a state described in the position basis rather than

the eigenbasis of A, it is necessary to be given sufficient information on the system to be able to derive the eigenvectors from the values λ_n and α_n. A chain is a particularly natural candidate and can be extended to chain-like systems [21, 22], although one could come up with many other variants

VI. CONCLUSIONS

In this paper, we have demonstrated how the capability of a spin network for state transfer can be computed, which has obvious potential bearing on the design of quantum information routers. All CSOs produce states which are robust to dephasing noise on the pendant control spins, and those for which catalysis fails (such as permutations) produce states which are robust to all noise on the pendant control spins. The difference between the two can be interpreted in terms of selection rules [23]: the selection rule preventing population of some states can be overcome by shifting to a different excitation subspace, but superselection rules prevent access to the truly dark states. This could direct the development of spin network memories in terms of decoherence-free subspaces, i.e. the dark states produced by the permutation symmetries of the excitation subspace graph could be used to store states. Truly dark states will be robust to the introduction of extra excitations in the system, but will need a corresponding permutation symmetry-breaking local control to enable their initialization and collection. The weaker class of dark states will be immediately vulnerable to the introduction of excitations elsewhere in the system; nevertheless they will be better protected than non-dark states and correspondingly easier to access using local controls than the truly dark states. The suitability of each method of storage will depend on the architecture employed and the relative importance placed on access and permanence. This is somewhat analogous to the relative advantages of RAM and ROM in conventional silicon computing.

We have seen how, in the pendant controlled spin networks, the necessary and sufficient condition for the existence of an ASO (on $\mathcal{H}_a$) is that the underlying graph should be bipartite. This link with the underlying graph structure is extremely interesting because it is much less artificial than previous studies which have found such a relation [12]. These studies imposed a direct relation between the Hamiltonian and the adjacency matrix of the graph by setting them equal, whereas our only constraint is that the graph structure specifies where coupling coefficients take on a non-zero value.

In the future it will be interesting to see when the state with optimal overlap can be achieved for arbitrary Hamiltonians, not just those with pendant controllers. A trivial extension of the present study is one where the graph A is composed of two connected components, and the control C couples between a single vertex of each of the two components. Further consequences of the control

required to introduce a state to transfer should also be examined [30].

VII. ACKNOWLEDGEMENTS

Appendix A: Identification of Symmetries

Given the Hamiltonian H_0 of an N-dimensional quantum system and its M control Hamiltonians H_m, it is relatively easy to determine the symmetries it possesses and thus limit the possible operations that can be realized. First we check for decomposability into a block-diagonal structure (i.e. we find the CSOs). This can be done by transforming each of the M Hamiltonians H_m from its $N \times N$ matrix representation into its Liouville representation, where it is represented by an $N^2 \times N^2$ matrix $L^{(m)}$ with entries

$$L_{s,r}^{(m)} := (H_m)_{n,k}\delta_{j,\ell} - (H_m)_{j,\ell}\delta_{n,k} \qquad \text{(A1)}$$

for $r = (j-1)N + k$ and $s = (\ell-1)N + n$. Repeating this for all system and control Hamiltonians H_m and stacking the resulting matrices $L^{(m)}$ vertically gives an $(M+1)N^2 \times N^2$ matrix. Any standard routine can be used to calculate the null space of this matrix, and the column vectors of length N^2 spanning the null space, "unstacked" into a $N \times N$ matrix, to give the CSOs J that simultaneously commute with all H_m, $[H_m, J] = 0$. This is a conceptually very simple approach. More efficient alternatives for simultaneous block-diagonalization such as the algorithm in [24], which requires handling matrices of lower dimension, exist.

To find the ASOs, we go through much the same procedure: for each indecomposable subspace, indexed by d, of each Hamiltonian H_m, we take the complexified system and control Hamiltonians restricted to the subspace, $iH_{m,d}$, remove the trace

$$\tilde{H}_{m,d} := iH_{m,d} - \text{Tr}(iH_{m,d})\frac{\mathbf{1}}{N}, \qquad \text{(A2)}$$

and compute the Liouvillian representation

$$\tilde{L}_{s,r}^{(m,d)} := (\tilde{H}_{m,d})_{n,k}\delta_{j,\ell} + (\tilde{H}_{m,d})_{j,\ell}\delta_{n,k}. \qquad \text{(A3)}$$

As before, we do this for all system and control Hamiltonians, stack the resulting Liouville operators, and calculate the null space of the resulting matrix. Unstacking the null vectors again results in ASOs $\tilde{J}$ such that $\tilde{H}_{m,d}^T\tilde{J} + \tilde{J}\tilde{H}_{m,d} = 0$ for all $\tilde{H}_{m,d}$. The ASOs $\tilde{J}$ define the possible superpositions within the subspaces spanned by the eigenvectors of the J CSOs. The eigenvalues of the $\tilde{J}$ may help identify the Lie subalgebras [25, 26].

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[31] For the initial studies which considered chains, this assumption was well motivated because there is no catalysis in this case.

[32] The term *globally controllable* is often coined here, as in [14]. However, we choose the alternative term to enable certain distinctions with, for instance, the subject that has come to be known as global control [27] that one of the authors has worked on [28], and the fact that full control can be realized with a single local coupling [5].

[33] Initialization using a local-interaction cooling method [29] can remove all excitations except for the dark states, and we can then catalytically reintroduce excitations to remove those dark states.

[34] If some coupling strengths are allowed to be negative, one can find counter-examples in which the weight on one loop can exactly cancel the weight on a second loop, such that the non-bipartite graph does have an ASO. These, however, are highly specialized cases.

[35] If it were not for the modulus in Eqn. (16), we could directly construct some of the symmetry operators in higher excitation subspaces directly from those in lower excitation subspaces, but this would make catalysis impossible. The only graph for which all these terms are positive anyway is the chain.

[36] Notice that $\alpha|0\rangle + \beta|\psi\rangle$ is a superposition of the zero-excitation state $|0\rangle$ and the state $|\psi\rangle$ in the single excitation subspace, and the relative phase of the superposition state is determined by the global phase of $|\psi\rangle$. This is a problem since we usually have limited control over the global phase of $|\psi\rangle$. This has been a perennial problem in the study of state transfer, and it is always assumed that one can simply correct for this phase difference with a local phase gate.